

Experimental NMR Realization of A Generalized Quantum Search Algorithm

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Abstract

A generalized quantum search algorithm, where phase inversions for the marked state and the prepared state are replaced by $\pi/2$ phase rotations, is realized in a 2-qubit NMR heteronuclear system. The quantum algorithm searches a marked state with a smaller step compared to standard Grover algorithm. Phase matching requirement in quantum searching is demonstrated by comparing it with another generalized algorithm where the two phase rotations are $\pi/2$ and $3\pi/2$ respectively. Pulse sequences which include non 90

degree pulses are given.

Grover's quantum search algorithm is one of the most important development in quantum computation [1]. It achieves quadratic speedup in searching a marked state in an unordered list over classical searching algorithms. It has many potential applications in various fields of interests, for instance in deciphering the DES encryption code [2] and algorithms that need searching. Typical examples of the algorithms that need searching are the Simon problem [3], the Hamilton's circuit problem [5], the hiddens shift problem [4] and quantum counting [6]. There are several generalizations of the Grover algorithm. A modification of the algorithm can search for a "chain" of m marked items in $O(\sqrt{N/m})$ iterations [7]. In the standard Grover algorithm, the quantum database is built on an evenly distributed quantum superposition, and a generalization is made to allow the algorithm to work on a biased database where the amplitudes of the items in a database are not even [8]. Searching in an arbitrary entangled superposition is given in Ref. [9]

In some cases, one needs a quantum searching engine that searches an item with a smaller step. For instance, in the Simon algorithm [3] where $\frac{\pi}{2}$ -phase rotations rather than phase inversions are used and in the case where the number of marked states is more than $N/4$ [10], standard Grover algorithm can not be used. In addition, for small N , state of the quantum computer may not be exactly the marked state during the search process, and there is small probability that the algorithm may fail. In problems that certainty of success is vital, this should be avoided. A generalized quantum search algorithm [11,12] suits this purpose, where the searching step can be anything between that of Grover algorithm and zero. This is done by replacing the two phase inversions in Grover's algorithm with smaller phase rotations(ϕ for phase rotation of the marked state, and θ for phase rotation of the prepared state $|0\dots0\rangle$). It has been found that with an evenly distributed database, arbitrary phase rotation is not applicable [11], and only when the two phase rotations satisfy the phase matching requirement $\theta = \phi$ that an efficient quantum searching algorithm can be constructed [12]. An approximate expression $2 \sin \frac{\theta}{2} \sqrt{\frac{1}{N}}$ was given for the search step [12], where θ is the rotation angle of the marked state [12]. Exact expressions are given in a $SO(3)$ geometric picture [13].

NMR implementation of Grover's algorithm has been realized in 2-qubit and 3-qubit systems [14,16,17]. Quantum counting has also been realized in NMR system [18]. Experimental studies are important in demonstrating quantum algorithms, investigating effects of gate imperfection and decoherence, and in identifying problems in building a practical quantum computer. In this Letter, we report the experimental realization of this phase matching quantum search algorithm where the phase inversions are replaced by rotations through $\pi/2$ in a 2 qubit heteronuclear system using NMR technique. To demonstrate the effect of phase matching, another experiment where $\theta = \pi/2$, $\phi = 3\pi/2$ is also performed. Different from standard Grover algorithm, the pulse sequences used here contain non 90 degree pulses, and the delay pulses need not be multiples of $\frac{1}{4J}$.

Grover algorithm consists of four steps in an iteration [7]: 1) a phase inversion of the marked state $I_\tau = I - 2|\tau\rangle\langle\tau|$; 2) the Walsh-Hadamard transformation W ; 3) a phase inversion of the prepared state $|0\rangle$, $I_0 = I - 2|0\rangle\langle 0|$; and 4) the Walsh-Hadamard transformation. The operator for one Grover iteration is $Q = -WI_0WI_\tau$. The steps 2-4 are combined to give the inversion about average D which has the following matrix

$$D_{ij} = W I_\tau W = \begin{cases} \frac{2}{N} & i \neq j \\ \frac{2}{N} - 1 & i = j \end{cases} \quad (1)$$

In the generalized quantum search algorithm, the phase inversions are replaced by arbitrary phase rotations. The corresponding operators, indicated by a "g" in the superscript, are

$$Q^g = D^g I_\tau^g = W I_0^g W I_\tau^g, \quad (2)$$

where

$$\begin{aligned} I_\tau^g &= I - (1 - e^{i\phi})|\tau\rangle\langle\tau|, \\ I_0^g &= I - (1 - e^{i\theta})|0\rangle\langle 0|, \\ D^g &= W I_0^g W. \end{aligned} \quad (3)$$

When $\theta = \phi = \pi$ the Grover algorithm is recovered. It is helpful to give the detailed expressions for a 2-qubit system. We assume that the marked state is $\tau = 3$. The operators are,

$$I_{\tau=3}^g = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}, \quad (4)$$

and

$$Q^g = W I_0^g W = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}. \quad (5)$$

For demonstration in this experiment, we choose $\theta = \phi = \pi/2$. In table I, we give the state vector for the quantum computer in each step during a quantum searching process where $|c\rangle = 1/\sqrt{N} \sum_{i \neq \tau} |i\rangle$. When phase matching requirement is not satisfied, the quantum algorithm will not work. To demonstrate this, we also give the state vectors of the quantum computer for the case with $\theta = \pi/2$ and $\phi = 3\pi/2$. Both algorithms are performed for 10 searching iterations. The probability for finding the marked state is the square of the coefficient of $|\tau\rangle$. These state vectors are converted to density matrices for comparisons with experiment.

In the experiment, the working media is H_2PO_3 . The 2 qubits are the nuclear spins of the H-atom and the P-atom. The observed J-coupling between 1H and ^{31}P is **647.451 Hz**. The experiment was performed on a Bruker 500 ARX NMR spectrometer. The frequencies for 1H (qubit A) and ^{31}P (qubit B) are 500MHz and 220MHz respectively. The Hamiltonian for this system can be modelled as a two-spin system with a weak coupling interaction,

$$H = \omega_A I_{AZ} + \omega_B I_{BZ} + 2\pi J_{AB} I_{AZ} I_{BZ}, \quad (6)$$

where $I_{AZ} = \frac{1}{2}\sigma_{ZA}$ is the angular momentum operator in the $\widehat{\mathbf{e}}_z$ direction for spin A. ω_A and ω_B describe the free precession frequencies of the nuclear spins A and B respectively. The magnetic field is in $-\widehat{\mathbf{e}}_z$ direction. The quantum gate operations needed in quantum computation can be constructed by a combination of some hard pulses and the delay pulses. Compared to the pulse sequences in the Grover algorithm for 2-qubit system, one needs only a small modification in the pulse sequences. First let's denote the following operators

$$\begin{aligned} X^\theta &= \exp[-i\theta I_x], \\ \overline{X^\theta} &= \exp[i\theta I_x], \\ Y^\theta &= \exp[-i\theta I_y], \\ \overline{Y^\theta} &= \exp[i\theta I_y], \end{aligned} \tag{7}$$

which are radio frequency(rf) pulses for rotations about \hat{x} -axis through θ , $-\theta$, rotations about \hat{y} -axis through θ and $-\theta$ respectively. In addition to these hard pulses, we also have

$$\tau^t = \exp[-2\pi i J_{AB} I_{ZA} I_{ZB} t],$$

which is a delay pulse where the system undergoes an evolution during period t in the doubly rotating frame. We denote $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$.

We used temporal averaging [19] to produce the effective pure state $|00\rangle$. The pulse sequences for the temporal averaging and the Hadmard-Walsh transformation are standard [14,15]:

$$\begin{aligned} P_0 &: I(\text{none}); \\ P1 &: Y_B^{\frac{\pi}{2}} \tau^{\frac{1}{2J}} X_B^{\frac{\pi}{2}} Y_A^{\frac{\pi}{2}} \tau^{\frac{1}{2J}} X_A^{\frac{\pi}{2}}, \\ P2 &: Y_A^{\frac{\pi}{2}} \tau^{\frac{1}{2J}} X_B^{\frac{\pi}{2}} X_A^{\frac{\pi}{2}} \tau^{\frac{1}{2J}} X_B^{\frac{\pi}{2}}, \\ W &= (X_A^{\frac{\pi}{2}})^2 \overline{Y_A^{\frac{\pi}{2}}} (X_B^{\frac{\pi}{2}})^2 \overline{Y_B^{\frac{\pi}{2}}}. \end{aligned}$$

The pulse sequences for the generalized quantum search algorithm are obtained by modifying the pulse sequences used for Grover's algorithm in Ref. [14]:

$$\begin{aligned}
I^g &= Y_A^{\frac{\pi}{2}} \overline{X_A^{\frac{\phi}{2}}} Y_A^{\frac{\pi}{2}} Y_B^{\frac{\pi}{2}} \overline{X_B^{\frac{\phi}{2}}} Y_B^{\frac{\pi}{2}} \tau^{\frac{2\pi-\phi}{2J\pi}}, \\
D^g &= Y_A^{\frac{\pi}{2}} X_A^{\frac{\theta}{2}} \overline{Y_A^{\frac{\pi}{2}}} Y_B^{\frac{\pi}{2}} X_B^{\frac{\theta}{2}} \overline{Y_B^{\frac{\pi}{2}}} \tau^{\frac{2\pi-\theta}{2J\pi}}.
\end{aligned} \tag{8}$$

The pulse sequence for a complete generalized search iteration $Q^g = D^g I^g$ is

$$Q^g = \overline{X_A^{\frac{\theta}{2}}} Y_A^{\frac{\pi}{2}} X_B^{\frac{\theta}{2}} Y_B^{\frac{\pi}{2}} \tau^{\frac{2\pi-\theta}{2J\pi}} X_A^{\frac{\phi}{2}} \overline{Y_A^{\frac{\pi}{2}}} X_B^{\frac{\phi}{2}} \overline{Y_B^{\frac{\pi}{2}}} \tau^{\frac{2\pi-\phi}{2J\pi}}. \tag{9}$$

It is interesting to study the length of time in a given quantum search algorithm with arbitrary phases. A hard pulse takes microsecond to complete while a delay pulse takes about a millisecond to complete. An algorithm with large θ or ϕ takes less time to complete. Therefore in practice, it is better to use large phase rotations to make the computation time short if one is given the freedom. It also worth pointing that in general, the hard pulses may not be the multiples of $\frac{\pi}{2}$ as in other NMR quantum computations, and the delay pulses may also takes noninteger multiples of $\frac{1}{4J}$. This is different from the pulse sequences used in standard Grover algorithm, for instance in [14,17].

Two sets of experiments: phase matched searching with $\theta = \phi = \frac{\pi}{2}$ and phase mismatched searching with $\theta = \frac{\pi}{2}, \phi = \frac{3\pi}{2}$, have been performed. State tomography is used to obtain the density matrices [20]. Density matrices are experimentally constructed for all the 10 iterations in the two sets of experiments. It took quite some time and labor to get them. In table II, we have given the relative error defined as $\delta\rho = \frac{\|\rho_{th} - \rho_{exp}\|_2}{\|\rho\|_2}$. However, this error is not solely the "genuine" errors [21,22] from gate imperfection and decoherence that occurs during the quantum computation process. Part of the error is caused by doing the integration of areas of the spectrum by hand during the density matrix construction. It is interesting to note that the relative errors at later stages are sometimes even smaller than the early stages. For instance at step 7 in the phase-matched case, the relative error is only 15% , the smallest among the 10 steps. Similar result is observed in other NMR quantum computing experiment, for instance in [14]. This is perhaps because imperfect gate errors cancel out each other. For the economy of the paper length, we give only the density matrix for the 6th iteration where the success rate is the largest in Fig.1 for phase matched searching. In Fig.2

the same is plotted for the phase mismatched searching. For clarity, we plot separately the real and imaginary parts. From these figures, it is seen that the agreement between theoretical prediction and experimental data is good. In particular, when phase matching is satisfied, the algorithm can find the marked state with high probability. However, when the phase matching requirement is seriously violated, the probability of finding the marked state is very low. Phase mismatching leads reduction in success rate, and it should be avoided in practice. However, Grover's algorithm has some intrinsic robustness against errors, a small amount of phase mismatching, like those errors from NMR pulse manipulations, will not cause a big loss in the probability for finding the marked state.

In summary, a generalized quantum search algorithm has been demonstrated in a 2-qubit NMR system. Pulse sequences are given. Non 90 degree pulses are used and tested to give good performance. It also demonstrate that phase matching in quantum searching is important.

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TABLES

TABLE I. Theoretical State Vector of the Register in Each Search Iteration

	phase matching $\theta = \phi = \pi/2$	phase mismatching $\theta = \pi/2, \phi = 3\pi/2$
step1:	$ \psi_1\rangle = 0.90 \tau\rangle + 0.43 c\rangle$	$ \psi_1\rangle = 0.25 \tau\rangle + 0.97 c\rangle$
step2:	$ \psi_2\rangle = 0.97 \tau\rangle + 0.22 c\rangle$	$ \psi_2\rangle = 0.62 \tau\rangle + 0.78 c\rangle$
step3:	$ \psi_3\rangle = 0.65 \tau\rangle + 0.76 c\rangle$	$ \psi_3\rangle = 0.06 \tau\rangle + 1.00 c\rangle$
step4:	$ \psi_4\rangle = 0.39 \tau\rangle + 0.92 c\rangle$	$ \psi_4\rangle = 0.59 \tau\rangle + 0.80 c\rangle$
step5:	$ \psi_5\rangle = 0.78 \tau\rangle + 0.62 c\rangle$	$ \psi_5\rangle = 0.36 \tau\rangle + 0.93 c\rangle$
step6:	$ \psi_6\rangle = 1.00 \tau\rangle + 0.01 c\rangle$	$ \psi_6\rangle = 0.41 \tau\rangle + 0.91 c\rangle$
step7:	$ \psi_7\rangle = 0.80 \tau\rangle + 0.60 c\rangle$	$ \psi_7\rangle = 0.57 \tau\rangle + 0.82 c\rangle$
step8:	$ \psi_8\rangle = 0.40 \tau\rangle + 0.92 c\rangle$	$ \psi_8\rangle = 0.13 \tau\rangle + 0.99 c\rangle$
step9:	$ \psi_9\rangle = 0.63 \tau\rangle + 0.77 c\rangle$	$ \psi_9\rangle = 0.63 \tau\rangle + 0.78 c\rangle$
step10:	$ \psi_{10}\rangle = 0.97 \tau\rangle + 0.24 c\rangle$	$ \psi_{10}\rangle = 0.19 \tau\rangle + 0.98 c\rangle$

TABLE II. The errors of the experiments

	$\theta = \phi = \frac{\pi}{2}$	$\theta = \frac{\pi}{2}, \phi = \frac{3\pi}{2}$
Step1	%18	%17
Step2	%21	%28
Step3	%20	%27
Step4	%21	%21
Step5	%27	%20
Step6	%20	%20
Step7	%15	%16
Step8	%24	%33
Step9	%22	%30
Step10	%22	%33

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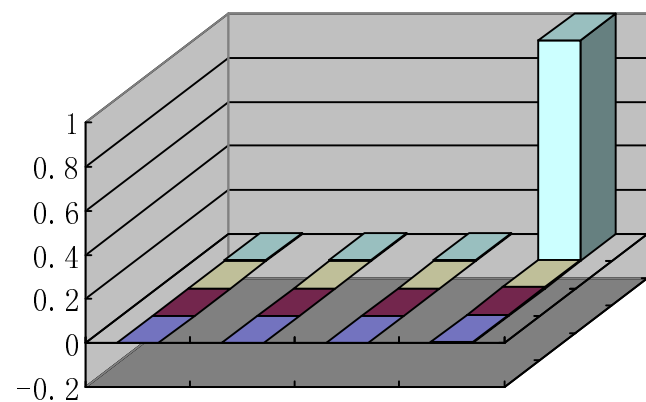
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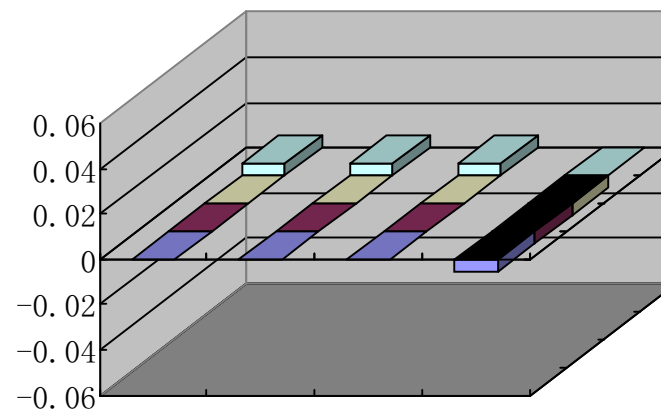
Figure captions

Fig.1 Comparisons of theoretical and experimental density matrices with $\theta = \phi = \pi/2$ for iteration 6. (a) and (b) are the theoretical real part and imaginary part of the density matrices respectively, whereas (c) and (d) are the corresponding experimental ones. The probability of finding the marked state is the sum of squares of the 11 component which are in the upper right corners of the figures.

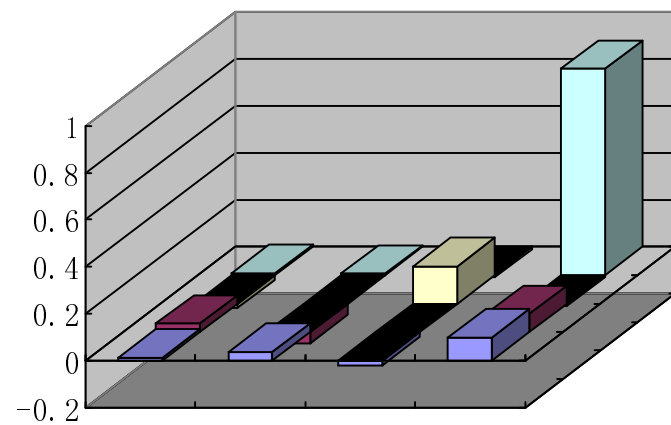
Fig.2 Same as Fig.2 but for $\theta = \pi/2, \phi = 3\pi/2$.



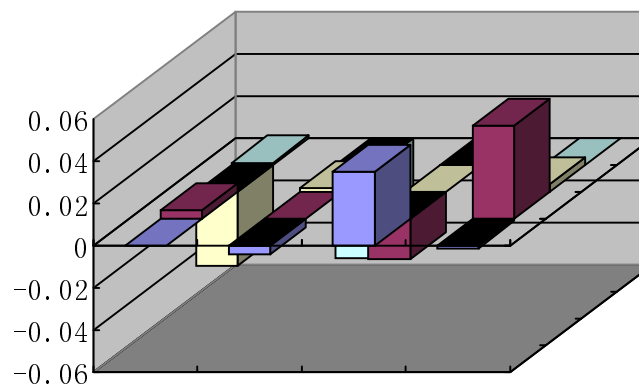
(a)



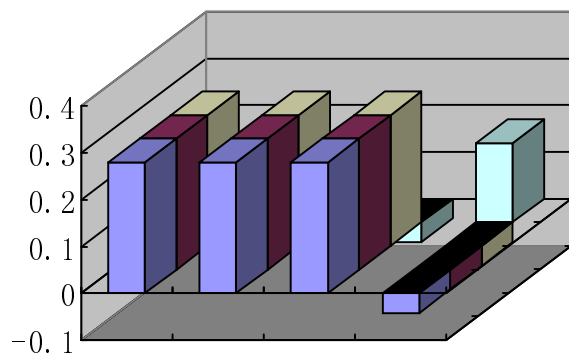
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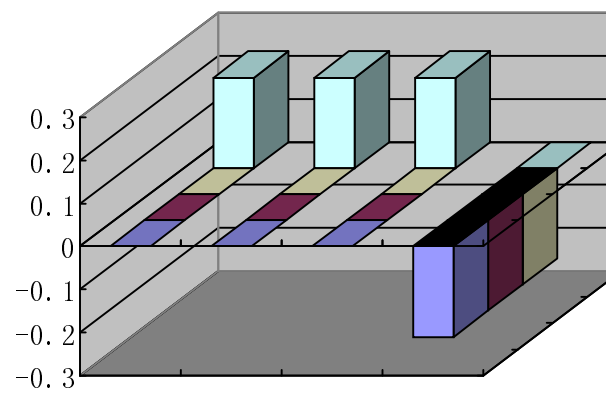
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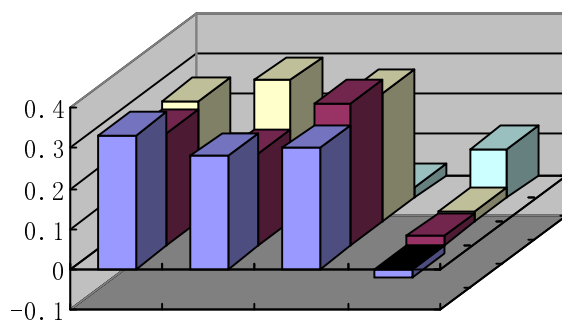
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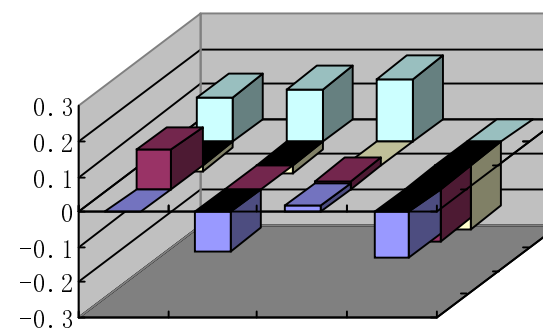
(a)



(b)



(c)



(d)